

Dihedral symmetry of periodic chain: quantization and coherent states

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Abstract. Our previous work on quantum kinematics and coherent states over finite configuration spaces is extended: the configuration space is, as before, the cyclic group \mathbf{Z}_n of arbitrary order $n = 2, 3, \dots$, but a larger group — the non-Abelian dihedral group \mathbf{D}_n — is taken as its symmetry group. The corresponding group related coherent states are constructed and their overcompleteness proved. Our approach based on geometric symmetry can be used as a kinematic framework for matrix methods in quantum chemistry of ring molecules.

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1. Introduction

The mathematical arena for ordinary quantum mechanics is, due to Heisenberg's commutation relations, the infinite-dimensional Hilbert space. A useful model for quantum mechanics in a Hilbert space of finite dimension n is due to H. Weyl [1]. Its geometric interpretation as the simplest quantum kinematic on a finite discrete configuration space formed by a periodic chain of n points, was elaborated by J. Schwinger [2]. In [3, 4] we proposed a group theoretical formulation of this quantum model in terms of Mackey's quantization [5, 6]. It is based on Mackey's system of imprimitivity which represents a group theoretical generalization of Heisenberg's commutation relations.

The geometrical picture behind the group theoretical approach is the following [7]: one has a discrete or continuous configuration space together with a geometrical symmetry group acting transitively on it, i.e. the configuration space is a homogeneous space of the group. In particular, Weyl's model is based on configuration space \mathbf{Z}_n (where \mathbf{Z}_n is the cyclic group of order $n = 2, 3, \dots$) with symmetry \mathbf{Z}_n acting on the periodic chain \mathbf{Z}_n by discrete translations. In this paper our formulation of Weyl's model is generalized by extending the Abelian symmetry group \mathbf{Z}_n of the periodic chain to the dihedral group \mathbf{D}_n — the non-Abelian symmetry group of a regular n -sided polygon.

Coherent states belong to the most important tools in many applications of quantum physics. They found numerous applications in quantum optics, quantum field

theory, condensed matter physics, atomic physics etc. There are various definitions and approaches to the coherent states dependent on author and application. Our main reference is [8], where the systems of coherent states related to Lie groups are described. The basic feature of such systems is that they are overcomplete. As shown for instance in [9], Perelomov's method can be equally well applied to discrete groups. Starting with irreducible systems of imprimitivity we shall construct irreducible sets of generalized Weyl operators, whose action on properly chosen vacuum states will produce the resulting families of coherent states.

In section 2 after recalling Mackey's Imprimitivity Theorem for finite groups [10] the construction of systems of imprimitivity is described. Then necessary notations for the dihedral groups are introduced in section 3. Section 4 is devoted to the construction of the two irreducible systems of imprimitivity for \mathbf{D}_n based on \mathbf{Z}_n , each consisting of a projection-valued measure and an induced unitary representation. From them, the corresponding quantum position and momentum observables are constructed in section 5. This is the starting point for construction of the set of generalized Weyl operators and generalized coherent states in section 6. We apply the method of paper [9], where quantization on \mathbf{Z}_n with Abelian symmetry group \mathbf{Z}_n and the corresponding coherent states were investigated. Concluding section 7 contains remarks concerning the replacement of the Abelian cyclic symmetry group \mathbf{Z}_n by the non-Abelian dihedral group \mathbf{D}_n as the group of motions of the configuration space \mathbf{Z}_n . The interesting feature of our construction is the fact that, even if the group property of the set of Weyl operators is lost, the families of coherent states still possess the required overcompleteness property.

2. Systems of imprimitivity for finite groups

We consider the case when the configuration space \mathbf{M} and its symmetry group \mathbf{G} are finite. Our configuration space will be a finite set $\mathbf{M} = \{m_1, m_2, \dots, m_n\}$, $n = |\mathbf{M}|$. Let \mathbf{G} be a finite group acting transitively on \mathbf{M} , and let \mathbf{H} be the stability subgroup. Let \mathbf{L} be an irreducible unitary representation of subgroup \mathbf{H} on Hilbert space $\mathcal{H}^{\mathbf{L}}$.

System of imprimitivity is a pair (\mathbf{V}, \mathbf{E}) , where \mathbf{E} is a projection-valued measure on configuration space \mathbf{G}/\mathbf{H} and \mathbf{V} is a unitary representation of the symmetry group \mathbf{G} such that

$$\mathbf{V}(g)\mathbf{E}(S)\mathbf{V}(g)^{-1} = \mathbf{E}(g.S) \quad \text{for all } g \in \mathbf{G}, S \subset \mathbf{G}/\mathbf{H}. \quad (1)$$

In a finite-dimensional Hilbert space $\mathcal{H} = \mathbb{C}^n$ the standard projection-valued measure is given by finite sums of diagonal matrices

$$\mathbf{E}(m_i) := \text{diag}(0, 0, \dots, 1, \dots, 0), \quad i = 1, 2, \dots, n. \quad (2)$$

The Imprimitivity Theorem for finite groups has the following form [10]:

Theorem : *A unitary representation \mathbf{V} of a finite group \mathbf{G} in Hilbert space \mathcal{H} belongs to the imprimitivity system (\mathbf{V}, \mathbf{E}) with standard projection-valued measure based on \mathbf{G}/\mathbf{H} , if and only if \mathbf{V} is equivalent to an induced representation $\text{Ind}_{\mathbf{H}}^{\mathbf{G}}(\mathbf{L})$ for some unitary representation \mathbf{L} of subgroup \mathbf{H} . The system of imprimitivity is irreducible, if and only if \mathbf{L} is irreducible.*

Thus a unitary representation \mathbf{V} for a system of imprimitivity is constructed directly as an induced representation. Let \mathbf{G} be a finite group of order r , \mathbf{H} its subgroup of order s . Suppose that \mathbf{L} is a representation of the subgroup \mathbf{H} . Let us decompose the group \mathbf{G} into left cosets

$$\mathbf{G} = \left\{ \bigcup_{j=1}^{r/s} t_j \cdot \mathbf{H} \mid t_j \in \mathbf{G}, t_1 = e \right\}. \quad (3)$$

Group elements t_j are arbitrarily chosen representatives of left cosets. If the dimension of the representation \mathbf{L} is l , then the induced representation \mathbf{V} of \mathbf{G} is given by

$$(\mathbf{V}(g))_{ij} = \mathbf{L}(h) \quad \text{if} \quad t_i^{-1} \cdot g \cdot t_j = h \quad \text{for some } h \in \mathbf{H}, \quad (4)$$

$$= 0 \quad \text{otherwise}; \quad (5)$$

here $(\mathbf{V}(g))_{ij}$ are $l \times l$ matrices which serve as building blocks for

$$\mathbf{V}(g) = \text{Ind}_{\mathbf{H}}^{\mathbf{G}}(\mathbf{L}) \quad (6)$$

and the subscript ij denotes the position of the block in $\mathbf{V}(g)$.

3. Structure of dihedral groups

The dihedral group \mathbf{D}_n , where $n = 2, 3, \dots$, is a non-Abelian finite group of order $2n$ with the structure of a semidirect product of two cyclic groups:

$$\mathbf{D}_n = \mathbf{Z}_n \rtimes \mathbf{Z}_2. \quad (7)$$

It arises as the symmetry group of a regular polygon and is generated by discrete rotations and reflections. The elements of the subgroups \mathbf{Z}_2 and \mathbf{Z}_n will be denoted

$$\mathbf{Z}_2 = \{+1, -1\}; \quad \mathbf{Z}_n = \{e = r_0, r_1, \dots, r_{n-1}\}. \quad (8)$$

Group operation in \mathbf{Z}_2 is multiplication, in \mathbf{Z}_n $r_i \cdot r_j = r_{i+j \pmod n}$.

The multiplication law of the semidirect product (7) is determined by a fixed homomorphism f from \mathbf{Z}_2 to the group of all automorphisms of the group \mathbf{Z}_n , $f : \mathbf{Z}_2 \rightarrow \text{Aut}(\mathbf{Z}_n)$:

$$(r_i, x) \cdot (r_j, y) = (r_i \cdot f(x)(r_j), x \cdot y), \quad x, y \in \mathbf{Z}_2, \quad r_i, r_j \in \mathbf{Z}_n. \quad (9)$$

Under this multiplication law, \mathbf{Z}_n is a normal subgroup. Specifically for \mathbf{D}_n , the mapping f is simply

$$f : +1 \mapsto \text{Id}, \quad f : -1 \mapsto \text{Inv}, \quad (10)$$

where Id is the identical mapping on \mathbf{Z}_n , Inv is an automorphism of \mathbf{Z}_n which maps an element of \mathbf{Z}_n into its inverse:

$$\text{Inv} : r_k \mapsto r_k^{-1} = r_{-k \pmod n}, \quad r_i \in \mathbf{Z}_n. \quad (11)$$

We shall need the explicit form of the multiplication law:

$$(r_i, +1) \cdot (r_j, x) = (r_i \cdot r_j, x) = (r_{i+j \pmod n}, x), \quad (12)$$

$$(r_i, -1) \cdot (r_j, x) = (r_i \cdot r_j^{-1}, -x) = (r_{i-j \pmod n}, -x). \quad (13)$$

Thus the elements of \mathbf{D}_n can be divided in two disjoint subsets:

- (i) The subset $\{(r_k, +1), k = 0, 1, \dots, n-1\}$ forms the subgroup isomorphic to \mathbf{Z}_n and the elements $(r_k, +1)$ have the geometrical meaning of integral multiples of a clockwise rotation of an n -sided regular polygon through an angle $2\pi/n$.
- (ii) The subset $\{(r_k, -1), k = 0, 1, \dots, n-1\}$ consists of mirror symmetries with respect to axes in the n -sided polygon: if n is odd, then all axes of mirror symmetries pass through vertices of the n -sided polygon; if n is even, then only one half of mirror symmetries have axes passing through opposite vertices, the remaining axes are symmetry axes of two opposite sides of the polygon.

Summarizing, the group \mathbf{D}_n consists of n rotation symmetries $\mathbf{R}_k = (r_k, +1)$ and n mirror symmetries $\mathbf{M}_k = (r_k, -1)$ obeying the following multiplication rules (with $i, j = 0, 1, \dots, n-1$):

$$\mathbf{R}_i \cdot \mathbf{R}_j = \mathbf{R}_{i+j \pmod n}, \quad \mathbf{R}_i \cdot \mathbf{M}_j = \mathbf{M}_{i+j \pmod n}, \quad (14)$$

$$\mathbf{M}_i \cdot \mathbf{R}_j = \mathbf{M}_{i-j \pmod n}, \quad \mathbf{M}_i \cdot \mathbf{M}_j = \mathbf{R}_{i-j \pmod n}. \quad (15)$$

4. Quantization on \mathbf{Z}_n with \mathbf{D}_n as a symmetry group

The configuration space \mathbf{Z}_n will be identified with the set of vertices of a regular n -sided polygon. We have seen that \mathbf{D}_n acts on \mathbf{Z}_n transitively as a group of discrete rotations and mirror symmetries. The stability subgroup \mathbf{H}_n of \mathbf{D}_n is \mathbf{Z}_2 for all n , hence we can write $\mathbf{Z}_n \cong \mathbf{D}_n/\mathbf{Z}_2$.

The stability subgroup \mathbf{Z}_2 is independent of the order of symmetry group \mathbf{D}_n and it has exactly two inequivalent irreducible unitary representations, the trivial representation

$$\mathbf{T}_1 : \mathbf{Z}_2 \rightarrow \mathbb{C} : \pm 1 \mapsto 1, \quad (16)$$

and the alternating representation

$$\mathbf{T}_2 : \mathbf{Z}_2 \rightarrow \mathbb{C} : +1 \mapsto +1, \quad -1 \mapsto -1. \quad (17)$$

Now the inequivalent quantum kinematics on the configuration space \mathbf{Z}_n are determined by inequivalent systems of imprimitivity on \mathbf{Z}_n with the symmetry group \mathbf{D}_n . We require irreducibility of systems of imprimitivity in order that the corresponding kinematical observables act irreducibly in the Hilbert space. There will be exactly two inequivalent irreducible systems of imprimitivity $(\mathbf{V}_1, \mathbf{E}_1)$ and $(\mathbf{V}_2, \mathbf{E}_2)$ with representations induced from irreducible unitary representations \mathbf{T}_1 and \mathbf{T}_2 .

In both cases the Hilbert space \mathcal{H} of quantum mechanics is the space of complex functions on the configuration space \mathbf{Z}_n and it is isomorphic to n -dimensional complex vector space \mathbb{C}^n with standard inner product

$$\langle z_1, z_2 \rangle = \sum_{i=0}^{n-1} \bar{z}_{1i} z_{2i}. \quad (18)$$

The standard projection-valued measure \mathbf{E} is common to both systems of imprimitivity $(\mathbf{V}_1, \mathbf{E})$ and $(\mathbf{V}_2, \mathbf{E})$. It is diagonal and generated by sums of one-dimensional orthogonal projectors on \mathbb{C}^n of the form

$$\mathbf{E}(r_i) = \begin{pmatrix} & & i & & \\ & & \cdot & & \\ \cdot & \cdot & 1 & \cdot & \cdot \\ & & \cdot & & \\ & & \cdot & & \end{pmatrix}, \quad i = 0, 1, \dots, n-1; \quad (19)$$

Measure of an empty set in \mathbf{Z}_n is the vanishing operator on \mathbb{C}^n , measure of the whole configuration space is the unit operator.

In order to obtain the two irreducible systems of imprimitivity, we shall construct the representations induced from \mathbf{T}_1 and \mathbf{T}_2 on \mathbb{C}^n ,

$$\mathbf{V}_1 = \text{Ind}_{\mathbf{Z}_2}^{\mathbf{D}_n}(\mathbf{T}_1), \quad \mathbf{V}_2 = \text{Ind}_{\mathbf{Z}_2}^{\mathbf{D}_n}(\mathbf{T}_2). \quad (20)$$

According to (3) the symmetry group \mathbf{D}_n is decomposed into left cosets,

$$\mathbf{D}_n = \left\{ \bigcup_{m=0}^{n-1} t_m \cdot \mathbf{Z}_2 \mid t_m \in \mathbf{D}_n, t_0 = e. \right\} \quad (21)$$

In our case we have $\mathbf{Z}_2 = \{\mathbf{R}_0, \mathbf{M}_0\}$; with the choice of coset representatives $t_m = \mathbf{R}_m$, $m = 0, 1, \dots, n-1$, we obtain the decomposition

$$\mathbf{D}_n = \{ \{\mathbf{R}_0, \mathbf{M}_0\} \cup \{\mathbf{R}_1, \mathbf{M}_1\} \cup \dots \cup \{\mathbf{R}_{n-1}, \mathbf{M}_{n-1}\} \}. \quad (22)$$

Matrices of induced representations are then constructed in block form: dimensions of both representations \mathbf{V}_1 and \mathbf{V}_2 are equal to n ,

$$\dim(\mathbf{V}_l) = \frac{|\mathbf{D}_n|}{|\mathbf{Z}_2|} \cdot \dim(\mathbf{T}_l) = \frac{2n}{2} \cdot 1 = n, \quad l = 1, 2, \quad (23)$$

and matrix elements (1×1 -blocks) have the following form:

$$\begin{aligned} \mathbf{V}_1(g)_{ij} &= \mathbf{T}_1(h) \quad \text{if } t_i^{-1} \cdot g \cdot t_j = h \quad \text{for some } h \in \mathbf{Z}_2, \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{24}$$

In our case $t_i = \mathbf{R}_i$, so the matrix element $(\mathbf{V}_i(g))_{ij}$ does not vanish if and only if

$$\mathbf{R}_{-i} \pmod{n} \cdot g \cdot \mathbf{R}_j \in \{\mathbf{R}_0, \mathbf{M}_0\}. \quad (25)$$

To construct the induced representation \mathbf{V}_1 — first for the subgroup of discrete rotations $g = \mathbf{R}_k$ — condition (25)

$$\mathbf{R}_{-i \pmod n} \cdot \mathbf{R}_k \cdot \mathbf{R}_j = \mathbf{R}_{-i+j+k \pmod n} \in \{\mathbf{R}_0, \mathbf{M}_0\} \quad (26)$$

is equivalent to $i = j + k \pmod{n}$, hence matrix elements (24) of discrete rotations are

$$(\mathbf{V}_1(\mathbf{R}_k))_{ij} = \delta_{i,j+k \pmod n}. \quad (27)$$

So the entire matrix is

$$\mathbf{V}_1(\mathbf{R}_k) =_k \begin{pmatrix} & & k & 1 & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & \ddots \\ & & & & & & \ddots \\ & & & & & & & 1 \\ 1 & & & & & & & \\ & 1 & & & & & & \\ & & \ddots & & & & & \\ & & & \ddots & & & & \\ & & & & 1 & & & \end{pmatrix}. \quad (28)$$

For the representation \mathbf{V}_1 of mirror symmetries $g = \mathbf{M}_k$ condition (25) acquires the form

$$\mathbf{R}_{-i \pmod n} \cdot \mathbf{M}_k \cdot \mathbf{R}_j = \mathbf{M}_{-i-j+k \pmod n} \in \{\mathbf{R}_0, \mathbf{M}_0\} \Leftrightarrow i = k - j \quad (29)$$

due to (14) - (15), so the matrix elements (24) of mirror symmetries are

$$(\mathbf{V}_1(\mathbf{M}_k))_{ij} = \delta_{i,k-j} \pmod n. \quad (30)$$

The matrix $\mathbf{V}_1(\mathbf{M}_k)$ has the explicit form

$$\mathbf{V}_1(\mathbf{M}_k) = \begin{pmatrix} & & & & & & 1 \\ & & & & \cdot & & \\ & k & & 1 & & & \\ & & \cdot & & & & \\ 1 & & & & & & \\ & & & & & & \\ & & & & & 1 & \\ & & & & & & \cdot \\ & & & & & & \\ & & & & \cdot & & \\ & & & 1 & & & \end{pmatrix} \quad (31)$$

The second representation \mathbf{V}_2 is obtained similarly via (24) as the representation induced from \mathbf{T}_2 with the result

$$\mathbf{V}_2(\mathbf{R}_k) = \mathbf{V}_1(\mathbf{R}_k), \quad \mathbf{V}_2(\mathbf{M}_k) = -\mathbf{V}_1(\mathbf{M}_k). \quad (32)$$

The representations \mathbf{V}_1 and \mathbf{V}_2 are unitary, reducible and inequivalent; as could be expected, the two systems of imprimitivity differ only on reflections in \mathbf{D}_n .

5. Quantum observables

The basic quantum observables — position and momentum operators — defining quantum kinematics on a configuration space have natural definition if a system of imprimitivity is given.

Classical position observable is a Borel mapping from the configuration space, in our case from \mathbf{Z}_n , to the set of real numbers. For the classical position observable counting the points in \mathbf{Z}_n ,

$$f : \mathbf{Z}_n \rightarrow \mathbb{R} : r_k \mapsto k, \quad k = 0, 1, \dots, n-1, \quad (33)$$

the corresponding *quantized position operator* $\hat{\mathbf{Q}}$ is expressed in terms of the projection-valued measure (19) as follows [7]:

$$\hat{\mathbf{Q}} := \sum_{k=0}^{n-1} k \cdot \mathbf{E}(f^{-1}(k)) = \sum_{k=0}^{n-1} k \cdot \mathbf{E}(r_k) = \text{diag}(0, 1, \dots, n-1). \quad (34)$$

Note that the position operator is the same for both systems of imprimitivity constructed in previous section, i.e. in both quantum kinematics.

In the continuous case, *quantized momentum operators* are obtained from unitary representation \mathbf{V} by means of Stone's theorem [11]: *To each one-parameter subgroup $\gamma(t)$ of a symmetry group there exists a self-adjoint operator $\hat{\mathbf{P}}$ such that*

$$\mathbf{V}(\gamma(t)) = \exp(-it\hat{\mathbf{P}}), \quad t \in \mathbb{R}. \quad (35)$$

However, this is not possible in the discrete case. One has to look for self-adjoint operators $\widehat{\mathbf{P}}_{1g}$ on \mathbb{C}^n such that

$$\mathbf{V}_1(g) = \exp(-i\widehat{\mathbf{P}}_{1g}), \quad l = 1, 2, \quad g \in \mathbf{D}_n. \quad (36)$$

One may try to compute the operators $\widehat{\mathbf{P}}_{1g}$ by inverting the exponential (36),

$$\widehat{\mathbf{P}}_{1g} = i \cdot \ln(\mathbf{V}_1(g)), \quad (37)$$

but then has to face the problem that the complex exponential is not invertible, so the operators $\widehat{\mathbf{P}}_{1g}$ will not be determined uniquely.

Computation of functions of matrices is possible via the Lagrange-Sylvester theorem (see the Appendix). However, the spectral data needed there have their own physical importance in quantum mechanics, so they will be determined below for the operators $\mathbf{V}_1(\mathbf{R}_k)$ and $\mathbf{V}_1(\mathbf{M}_k)$, $k = 0, 1, \dots, n-1$. Because of (32) they are applicable to the other system of imprimitivity, too.

Let us start with discrete rotations. The eigenvalues of operator $\mathbf{V}_1(\mathbf{R}_1)$ are solutions of the secular equation

$$\det(\lambda \mathbb{I} - \mathbf{V}_1(\mathbf{R}_1)) = 0 \quad \text{or} \quad \lambda^n - 1 = 0, \quad (38)$$

hence the spectrum is

$$\sigma(\mathbf{V}_1(\mathbf{R}_1)) = \{\lambda_j = e^{\frac{2\pi i j}{n}} | j = 0, 1, \dots, n-1\}. \quad (39)$$

Then the eigenvalues of operators $\mathbf{V}_1(\mathbf{R}_k)$ are simply the powers of those of $\mathbf{V}_1(\mathbf{R}_1)$,

$$\sigma(\mathbf{V}_1(\mathbf{R}_k)) = \sigma(\mathbf{V}_1((\mathbf{R}_1)^k)) = \{\lambda_j^k = e^{\frac{2\pi i j k}{n}} | j = 0, 1, \dots, n-1\}. \quad (40)$$

Similarly the spectra of operators $\mathbf{V}_1(\mathbf{M}_k)$ for mirror symmetries are obtained by solving

$$\det(\lambda \mathbb{I} - \mathbf{V}_1(\mathbf{M}_k)) = 0, \quad (41)$$

but here two cases should be distinguished.

(i) If n is *odd*, then (41) becomes

$$(1 - \lambda)(\lambda^2 - 1)^{\frac{n-1}{2}} = 0 \quad \Rightarrow \quad \sigma(\mathbf{V}_1(\mathbf{M}_k)) = \{+1, -1\} \quad (42)$$

and the multiplicities of eigenvalues ± 1 are $\frac{n \pm 1}{2}$.

(ii) If n is *even*, then the characteristic polynomial of operator $\mathbf{V}_1(\mathbf{M}_k)$ depends, in addition to dimension n , also on parameter k . At this point we have also to distinguish if k is odd or even. In the geometric picture we have to distinguish if the axis of mirror symmetry \mathbf{M}_k passes through opposite vertices of the n -sided regular polygon (k even), or if it is an axis of two opposite sides of the polygon (k odd). So if n is even, then (41) has following form:

$$0 = (1 - \lambda)^{\frac{n}{2}+1} (1 + \lambda)^{\frac{n}{2}-1} \text{ if } k \text{ is even,} \quad (43)$$

$$0 = (1 - \lambda)^{\frac{n}{2}} (1 + \lambda)^{\frac{n}{2}} \text{ if } k \text{ is odd.} \quad (44)$$

The spectra for both cases are the same as for odd n , but the multiplicities of eigenvalues are different. If k is even, the multiplicity of eigenvalue $+1$ is $\frac{n}{2} + 1$, the multiplicity of eigenvalue -1 is $\frac{n}{2} - 1$; if k is odd, then the multiplicity of both eigenvalues is $\frac{n}{2}$.

The evaluation of operators $\widehat{\mathbf{P}}_{1\mathbf{R}_k}$ for discrete rotations can be done using the fact that rotations \mathbf{R}_k form an Abelian subgroup \mathbf{Z}_n of \mathbf{D}_n . Thus we have simply

$$\exp(-i\widehat{\mathbf{P}}_{\mathbf{R}_k}) = \mathbf{V}_1(\mathbf{R}_k) = (\mathbf{V}_1(\mathbf{R}_1))^k = \exp(-ik\widehat{\mathbf{P}}) \quad (45)$$

where $\widehat{\mathbf{P}} = \widehat{\mathbf{P}}_{1\mathbf{R}_1}$ can be interpreted as self-adjoint momentum operator. The spectrum (40) of $\mathbf{V}_1(\mathbf{R}_1)$ has n different simple eigenvalues $\lambda_k = e^{\frac{2\pi i k}{n}}$, so it remains to find the corresponding one-dimensional spectral projectors

$$\mathbb{P}_k = |k\rangle\langle k|. \quad (46)$$

Here $|k\rangle$ are normalized eigenvectors of operator $\mathbf{V}_1(\mathbf{R}_1)$ belonging to eigenvalues λ_k [4]:

$$|k\rangle = \frac{1}{\sqrt{n}} \begin{pmatrix} \lambda_k^{n-1} \\ \lambda_k^{n-2} \\ \vdots \\ \lambda_k \\ 1 \end{pmatrix}, \quad (47)$$

Using (46), matrix elements of \mathbb{P}_k can be written as

$$(\mathbb{P}_k)_{lm} = \frac{1}{n} \lambda_k^{n-l} \overline{\lambda_k^{n-m}} = \frac{1}{n} e^{\frac{2\pi i k(m-l)}{n}}. \quad (48)$$

Then, using (37) for simple eigenvalues, we have

$$(\widehat{\mathbf{P}})_{lm} = i(\ln \mathbf{V}_1(\mathbf{R}_1))_{lm} = i \sum_{j=0}^{n-1} \ln(\lambda_j) (\mathbb{P}_j)_{lm}, \quad (49)$$

hence matrix elements of the momentum operator are obtained:

$$(\widehat{\mathbf{P}})_{lm} = \frac{2\pi}{n} \frac{1}{1 - e^{\frac{2\pi i(m-l)}{n}}} \quad m \neq l, \quad (50)$$

$$= -\pi \frac{n-1}{n} \quad m = l. \quad (51)$$

Note that this result was obtained in [9] by finite Fourier transform of the position operator. For the analysis of operators of mirror symmetries see the Appendix. From the physical point of view unitary operators $\mathbf{V}_{1,2}(\mathbf{M}_k)$ play the role of parity operators.

6. Coherent states parametrized by $\mathbf{Z}_n \times \mathbf{D}_n$

In this section generalized coherent states will be determined for each of the two quantum kinematics.

A family of generalized coherent states of type $\{\Gamma(g), |\psi_0\rangle\}$ in the sense of Perelomov [8] is defined for a representation $\Gamma(g)$ of a group \mathbf{G} as a family of states $\{|\psi_g\rangle\}$, $|\psi_g\rangle = \Gamma(g)|\psi_0\rangle$, where g runs over the whole group \mathbf{G} and $|\psi_0\rangle$ is the ‘vacuum’ vector.

First take quantum kinematics defined by the system of imprimitivity $(\mathbf{V}_1, \mathbf{E})$. To construct group-related coherent states of Perelomov type parametrized by $(a, g) \in \mathbf{Z}_n \times \mathbf{D}_n$, we define generalized Weyl operators

$$\widehat{\mathbf{W}}_1(a, g) = \exp\left(\frac{2\pi ia}{n} \widehat{\mathbf{Q}}\right) \exp(-i \widehat{\mathbf{P}}_{1g}) = e^{\frac{2\pi ia}{n} \widehat{\mathbf{Q}}} \mathbf{V}_1(g); \quad a \in \mathbf{Z}_n, g \in \mathbf{D}_n. \quad (52)$$

Here

$$(e^{\frac{2\pi ia}{n} \widehat{\mathbf{Q}}})_{jk} = \delta_{j,k} e^{\frac{2\pi iaj}{n}}, \quad \exp\left(\frac{2\pi ia}{n} \widehat{\mathbf{Q}}\right) = \begin{pmatrix} 1 & & & \\ & e^{2\pi \frac{ia}{n}} & & \\ & & \ddots & \\ & & & e^{\frac{2\pi ia(n-1)}{n}} \end{pmatrix}. \quad (53)$$

Note that, if the system of imprimitivity is irreducible, also the set of generalized Weyl operators defined above acts irreducibly in the Hilbert space \mathcal{H} . Restricting g to the subgroup \mathbf{Z}_n of discrete rotations, the unitary operators satisfy

$$e^{\frac{2\pi ia}{n} \widehat{\mathbf{Q}}} e^{im \widehat{\mathbf{P}}} = e^{\frac{2\pi iam}{n}} e^{im \widehat{\mathbf{P}}} e^{\frac{2\pi ia}{n} \widehat{\mathbf{Q}}} \quad (54)$$

and operators $\widehat{\mathbf{W}}_1(a, g)$ form the well-known projective unitary representation of the group $\mathbf{Z}_n \times \mathbf{Z}_n$, which acts irreducibly in the Hilbert space $\mathcal{H} = \mathbb{C}^n$ [1, 4].

Unfortunately, if we want to derive a relation similar to (54) for operators $\widehat{\mathbf{P}}_{1\mathbf{M}_k}$, by performing the same computation as for $\widehat{\mathbf{P}}$ we obtain

$$(e^{\frac{2\pi ia}{n} \widehat{\mathbf{Q}}} e^{i \widehat{\mathbf{P}}_{1\mathbf{M}_m}})_{jk} = e^{\frac{2\pi ia}{n} (2m-2k)} (e^{i \widehat{\mathbf{P}}_{1\mathbf{M}_m}} e^{\frac{2\pi ia}{n} \widehat{\mathbf{Q}}})_{jk}. \quad (55)$$

Here the multiplier is k -dependent, hence there is neither an operator equality similar to (54) nor a projective representation property of operators $\widehat{\mathbf{W}}_1(a, g)$.

To construct the system of coherent states in \mathbb{C}^n , besides the system of operators $\widehat{\mathbf{W}}_1(a, g)$ a properly defined ‘vacuum’ vector $|0\rangle$ is needed. Then generalized coherent states of type $\{\widehat{\mathbf{W}}_1(a, g), |0\rangle\}$ are given by

$$|a, g\rangle_1 = \widehat{\mathbf{W}}_1(a, g)|0\rangle, \quad a \in \mathbf{Z}_n, g \in \mathbf{D}_n, \quad (56)$$

and $|0\rangle = |0, e\rangle_1$. In analogy with continuous case where the coherent states are eigenvectors of the annihilation operator and the vacuum vector belongs to eigenvalue 0 one would like to have a similar condition [9]

$$e^{\frac{2\pi}{n}\widehat{\mathbf{Q}}}e^{i\widehat{\mathbf{P}}}|0\rangle = |0\rangle. \quad (57)$$

But (57) cannot hold true since 1 is not an eigenvalue of the operator. So our admissible vacuum vectors are required to satisfy (57) up to a non-zero multiplier [9],

$$e^{\frac{2\pi}{n}\widehat{\mathbf{Q}}}e^{i\widehat{\mathbf{P}}}|0\rangle = \lambda|0\rangle. \quad (58)$$

For n spectral values

$$\sigma(e^{\frac{2\pi}{n}\widehat{\mathbf{Q}}}e^{i\widehat{\mathbf{P}}}) = \{\lambda_k = e^{\frac{\pi(n-1)}{n}}e^{\frac{2\pi ik}{n}} \mid k = 0, 1, \dots, n-1\} \quad (59)$$

we obtain a system of n admissible (normalized) vacuum vectors $|0\rangle^{(k)}$ labeled by $k = 0, 1, \dots, n-1$,

$$|0\rangle^{(k)} = \mathcal{A}_n \begin{pmatrix} 1 \\ e^{\frac{\pi(3-n)}{n}}e^{\frac{-2\pi ik}{n}} \\ \vdots \\ e^{\frac{\pi(n-1)}{n}}e^{\frac{-2\pi ik(n-1)}{n}} \end{pmatrix}; \quad (60)$$

here the j -th component

$$(|0\rangle^{(k)})_j = g_j^{(k)} = \mathcal{A}_n e^{\frac{\pi j(j-n+2)}{n}} e^{-j\frac{2\pi ik}{n}}, \quad (61)$$

where $j = 0, 1, \dots, n-1$ and \mathcal{A}_n is the normalization constant

$$\mathcal{A}_n = \frac{1}{\sqrt{\sum_{j=0}^{n-1} e^{\frac{2\pi}{n}j(j-n+2)}}}. \quad (62)$$

Now we are able to construct n families of coherent states in the first quantum kinematics which are labeled by parameter k . Applying (56) for \mathbf{R}_m , we obtain

$$\begin{aligned} (|a, \mathbf{R}_m\rangle_1^{(k)})_j &= (\widehat{\mathbf{W}}_1(a, \mathbf{R}_m)|0\rangle^{(k)})_j = \\ &= (e^{\frac{2\pi ia}{n}\widehat{\mathbf{Q}}}\widehat{\mathbf{V}}_1(\mathbf{R}_m)|0\rangle^{(k)})_j = e^{\frac{2\pi ia j}{n}} g_{j-m \pmod{n}}^{(k)}; \end{aligned} \quad (63)$$

for \mathbf{M}_m we obtain

$$\begin{aligned} (|a, \mathbf{M}_m\rangle_1^{(k)})_j &= (\widehat{\mathbf{W}}_1(a, \mathbf{M}_m)|0\rangle^{(k)})_j = \\ &= (e^{\frac{2\pi ia}{n}\widehat{\mathbf{Q}}}\widehat{\mathbf{V}}_1(\mathbf{M}_m)|0\rangle^{(k)})_j = e^{\frac{2\pi ia j}{n}} g_{m-j \pmod{n}}^{(k)}. \end{aligned} \quad (64)$$

Coherent states for the second quantum mechanics with representation \mathbf{V}_2 are equivalent to those of the first one because they differ on \mathbf{M}_m by an unessential phase factor -1 :

$$|a, \mathbf{R}_m\rangle_2^{(k)} = |a, \mathbf{R}_m\rangle_1^{(k)}, \quad |a, \mathbf{M}_m\rangle_2^{(k)} = -|a, \mathbf{M}_m\rangle_1^{(k)}. \quad (65)$$

7. Properties of coherent states

One of the most important properties of coherent states is their overcompleteness expressed by a resolution of unity

$$\sum_{(a,g) \in \mathbf{Z}_n \times \mathbf{D}_n} |a, g\rangle^{(k)} \langle a, g|^{(k)} = c_k \hat{\mathbb{I}}, \quad (66)$$

where c_k is some non-zero complex number. Let us check this property for our coherent states. From (63) and (64) we get

$$\begin{aligned} \sum_{(a,g) \in \mathbf{Z}_n \times \mathbf{D}_n} |a, g\rangle_{1,2}^{(k)} \langle a, g|_{1,2}^{(k)} &= \sum_{a \in \mathbf{Z}_n, m=0, \dots, n-1} |a, \mathbf{R}_m\rangle_1^{(k)} \langle a, \mathbf{R}_m|_1^{(k)} \\ &+ \sum_{a \in \mathbf{Z}_n, m=0, \dots, n-1} |a, \mathbf{M}_m\rangle_1^{(k)} \langle a, \mathbf{M}_m|_1^{(k)}. \end{aligned} \quad (67)$$

Matrix element of the first sum on the right-hand side of (67) is, due to (61) and (62),

$$\begin{aligned} \left(\sum_{a,m} |a, \mathbf{R}_m\rangle_1^{(k)} \langle a, \mathbf{R}_m|_1^{(k)} \right)_{jl} &= \sum_{a,m} (|a, \mathbf{R}_m\rangle_1^{(k)})_j (\langle a, \mathbf{R}_m|_1^{(k)})_l = \\ &= \sum_{a,m} e^{\frac{2\pi i a}{n}(j-l)} g_{j-m}^{(k)} \overline{g_{l-m}^{(k)}} \pmod{n} = n \delta_{j,l} \langle 0|0\rangle^{(k)} = n \delta_{j,l}. \end{aligned} \quad (68)$$

Exactly the same result is obtained for the second sum on the right-hand side of (67):

$$\begin{aligned} \left(\sum_{a,m} |a, \mathbf{M}_m\rangle_1^{(k)} \langle a, \mathbf{M}_m|_1^{(k)} \right)_{jl} &= \sum_{a,m} e^{\frac{2\pi i a}{n}(j-l)} g_{m-j}^{(k)} \overline{g_{m-l}^{(k)}} \pmod{n} = \\ &= n \delta_{j,l} \sum_m g_{m-j}^{(k)} \overline{g_{m-l}^{(k)}} \pmod{n} = n \delta_{j,l}. \end{aligned} \quad (69)$$

So we have proved that the resolution of unity is fulfilled:

$$\sum_{(a,g) \in \mathbf{Z}_n \times \mathbf{D}_n} |a, g\rangle_{1,2}^{(k)} \langle a, g|_{1,2}^{(k)} = 2n \hat{\mathbb{I}} \quad (70)$$

and this result holds for both representations \mathbf{V}_1 and \mathbf{V}_2 .

For the inner product (overlap) of two coherent states we have the formulae

$$\begin{aligned} \langle a, \mathbf{R}_p | b, \mathbf{R}_q \rangle_{1,2}^{(k)} &= \sum_{j=1}^n e^{\frac{2\pi i j}{n}(b-a)} \overline{g_{j-p}^{(k)}} g_{j-q}^{(k)} \pmod{n}, \\ \langle a, \mathbf{M}_p | b, \mathbf{M}_q \rangle_{1,2}^{(k)} &= \sum_{j=1}^n e^{\frac{2\pi i j}{n}(b-a)} \overline{g_{p-j}^{(k)}} g_{q-j}^{(k)} \pmod{n}, \\ \langle a, \mathbf{R}_p | b, \mathbf{M}_q \rangle_{1,2}^{(k)} &= \sum_{j=1}^n e^{\frac{2\pi i j}{n}(b-a)} \overline{g_{j-p}^{(k)}} g_{q-j}^{(k)} \pmod{n}. \end{aligned} \quad (71)$$

Note that the inner products yield the reproducing kernel $\langle x|x' \rangle = K(x, x')$ [12].

If the system is prepared in the coherent state $|a, g\rangle_{1,2}^{(k)}$, then the probability to measure the eigenvalue j of position operator is given by $|\langle j|a, g\rangle_{1,2}^{(k)}|^2$. It is independent of k and is the same in both quantum kinematics, namely,

$$\begin{aligned} |\langle j|a, \mathbf{R}_m\rangle_{1,2}^{(k)}|^2 &= \mathcal{A}_n^2 e^{\frac{2\pi}{n}(j-m)(j-m-n+2)}, \\ |\langle j|a, \mathbf{M}_m\rangle_{1,2}^{(k)}|^2 &= \mathcal{A}_n^2 e^{\frac{2\pi}{n}(m-j)(m-j-n+2)}. \end{aligned} \quad (72)$$

8. Concluding remarks

In this paper we have constructed systems of imprimitivity on the finite configuration space \mathbf{Z}_n considered as a homogeneous space of the dihedral group \mathbf{D}_n . We have shown that there exist two inequivalent irreducible systems of imprimitivity $(\mathbf{V}_1, \mathbf{E})$ and $(\mathbf{V}_2, \mathbf{E})$. Unitary representations \mathbf{V}_1 and \mathbf{V}_2 have clear physical significance of symmetry transformations.

Using these systems of imprimitivity, we have constructed the corresponding families of group related coherent states in the sense of Perelomov. They are connected with the group $\mathbf{Z}_n \times \mathbf{D}_n$ acting on the discrete phase space $\mathbf{Z}_n \times \mathbf{Z}_n$. Unfortunately, due to (55) we have lost the group property of the set of operators $\widehat{\mathbf{W}}(a, g)$, i.e. these operators do not form a projective unitary representation of the group $\mathbf{Z}_n \times \mathbf{D}_n$. In spite of this fact for the first system of imprimitivity n families of coherent states were obtained, generated from n admissible vacuum vectors (61). It turned out that the coherent states for the second system of imprimitivity differ from the first only by an unessential phase factor, i.e., they are physically equivalent. For all n families of coherent states the overcompleteness property was demonstrated. We have also evaluated the overlaps of pairs of coherent states in the form of finite sums (71). The only physical difference between the two quantum kinematics can be observed in the difference between unitary representations \mathbf{V}_1 and \mathbf{V}_2 on mirror symmetries, which have the meaning of parity operators.

Let us note that in quantum optics, discrete phase space $\mathbf{Z}_n \times \mathbf{Z}_n$ is employed in connection with the quantum description of phase conjugated to number operator [13]. Our approach can also provide a suitable starting point for the approximate solution of the continuous Schrödinger equation. In this connection we found instructive the paper [14] on finite approximation of continuous Weyl systems inspired by an approximation scheme due to J. Schwinger [15].

Another interesting application is offered by quantum chemistry, viz. Hückel's treatment of delocalized π -electrons and its generalizations in various kinds of molecules, where molecular orbitals are expressed as linear combinations of atomic orbitals [16, 17]. In this respect our approach seems especially suitable for the treatment of ring molecules with n equivalent carbon atoms called annulenes. In our notation, the set of atomic orbitals would correspond to the standard basis in $\mathcal{H} = \mathbb{C}^n$ and unitary representations \mathbf{V}_1 and \mathbf{V}_2 realize the geometric symmetry transformations.

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Appendix

For computation of matrix functions the Lagrange–Sylvester theorem is useful:

Theorem [18]. *Let \mathbb{A} be an $n \times n$ matrix with spectrum $\sigma(\mathbb{A}) = \{\lambda_1, \lambda_2, \dots, \lambda_s\}$, $s \leq n$. Let q_j be the multiplicity of eigenvalue λ_j , $j = 1, 2, \dots, s$. Let $\Omega \subset \mathbb{C}$ be an open subset*

of the complex plane such that $\sigma(\mathbb{A}) \subset \Omega$. Then the formula

$$f(\mathbb{A}) = \sum_{j=1}^s \sum_{k=0}^{q_j-1} \frac{f^{(k)}(\lambda_j)}{k!} (\mathbb{A} - \lambda_j \mathbb{I})^k \mathbb{P}_j \quad (73)$$

holds for every function f holomorphic on Ω . Here \mathbb{P}_j is the orthogonal projector onto the subspace of \mathbb{C}^n which is spanned by the set of all eigenvectors with eigenvalue λ_j :

$$\mathbb{P}_j := \prod_{l=1, l \neq j}^s \frac{\lambda_l \mathbb{I} - \mathbb{A}}{\lambda_l - \lambda_j}. \quad (74)$$

The formula (73) can be applied to equation (37) to evaluate operators $\widehat{\mathbf{P}}_{\mathbf{1}_g}$ for mirror symmetries. Since the multiplicities of spectral values ± 1 have already been determined, we have only to find the spectral projectors \mathbb{P}_k for each representation element $\mathbf{V}_1(\mathbf{M}_k)$. From equation (37)

$$\widehat{\mathbf{P}}_{\mathbf{1}_{\mathbf{M}_k}} = i \cdot \ln(\mathbf{V}_1(\mathbf{M}_k)), \quad (75)$$

we get, using the Lagrange–Sylvester formula (73) with spectrum (42), the spectral decomposition

$$\begin{aligned} \widehat{\mathbf{P}}_{\mathbf{1}_{\mathbf{M}_k}} &= i \cdot \sum_{j=0}^{q_{(+)}-1} \frac{\ln^{(j)}(+1)}{j!} (\mathbf{V}_1(\mathbf{M}_k) - \mathbb{I})^j \widehat{\mathbb{P}}_{+1} \\ &+ i \cdot \sum_{j=0}^{q_{(-)}-1} \frac{\ln^{(j)}(-1)}{j!} (\mathbf{V}_1(\mathbf{M}_k) + \mathbb{I})^j \widehat{\mathbb{P}}_{-1}, \end{aligned} \quad (76)$$

where $q_{(\pm)}$ are multiplicities of eigenvalues ± 1 . Strictly said the assumption of the Lagrange–Sylvester formula (73) is not satisfied since the complex logarithm is not holomorphic on the non-positive part of the real axis and -1 belongs to the spectrum of $\mathbf{V}_1(\mathbf{M}_k)$. We will express $\widehat{\mathbf{P}}_{\mathbf{M}_k}$ in a formal way and verify (36) using (73), where function exp is holomorphic.

Using formula (74) for the projectors projecting on $q_{(\pm)}$ -dimensional subspaces of \mathbb{C}^n

$$\widehat{\mathbb{P}}_{+1} = \frac{(\mathbf{V}_1(\mathbf{M}_k) + \mathbb{I})}{2}, \quad \widehat{\mathbb{P}}_{-1} = -\frac{(\mathbf{V}_1(\mathbf{M}_k) - \mathbb{I})}{2}, \quad (77)$$

and the property

$$(\mathbf{V}_1(\mathbf{M}_k) - \mathbb{I})(\mathbf{V}_1(\mathbf{M}_k) + \mathbb{I}) = (\mathbf{V}_1(\mathbf{M}_k))^2 - \mathbb{I} = \widehat{0}, \quad (78)$$

all elements in the sum (76) vanish except $j = 0$:

$$\widehat{\mathbf{P}}_{\mathbf{1}_{\mathbf{M}_k}} = i \cdot \left(\frac{\ln(+1)}{2} (\mathbf{V}_1(\mathbf{M}_k) + \mathbb{I}) - \frac{\ln(-1)}{2} (\mathbf{V}_1(\mathbf{M}_k) - \mathbb{I}) \right). \quad (79)$$

Taking the value $-\pi$ for $\ln(-1)$

$$\widehat{\mathbf{P}}_{\mathbf{1}_{\mathbf{M}_k}} = \frac{\pi}{2} (\mathbf{V}_1(\mathbf{M}_k) - \mathbb{I}); \quad (80)$$

similar calculation leads to

$$\widehat{\mathbf{P}}_{\mathbf{2}_{\mathbf{M}_k}} = \frac{\pi}{2} (\mathbf{V}_2(\mathbf{M}_k) - \mathbb{I}). \quad (81)$$

Note that momentum operators are not uniquely determined. This is caused by the property of exponential mapping which is not one-to-one.

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